Simplifying the Design of Workflows for Large-Scale Data Exploration and Visualization

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Workflows and Computational Processes

- Workflows are emerging as a paradigm for representing and managing complex computations
  - Simulations, data analysis, visualization, data integration
- They capture computation and analysis processes, enabling
  - Automation, reproducibility, result sharing
- Workflows are rapidly replacing primitive *shell* scripts
  - Apple's Mac OS X Automator, Microsoft Windows Workflow Foundation, and Yahoo! Pipes
- Business Workflows ⇒ Scientific Workflows
  - Important differences!

Workflows: Scientific vs. Business

- Express sequence of data transformations
- Dataflow: Stateless, functional
- Data intensive, computing intensive
- Cater to a broad set of users

- Ensure rules and prescribed processes are followed
- Control flow (e.g., BPEL): State and side effects
- Targeted to programmers

Exploration and Workflows

- Workflows have been traditionally used to automate repetitive tasks
- In exploratory tasks, *change is the norm*!
  - Data analysis and exploration are iterative processes

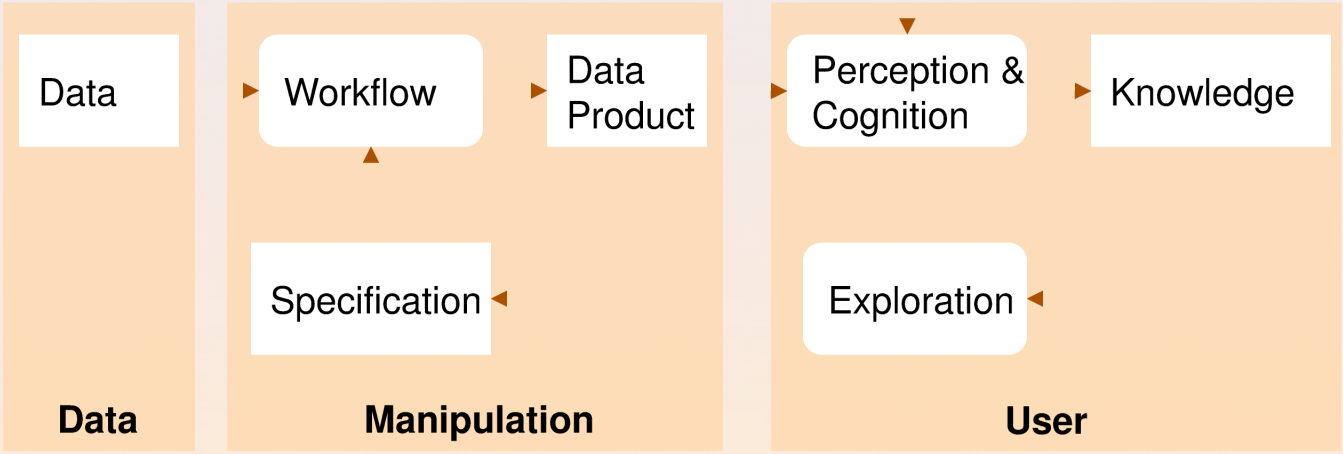
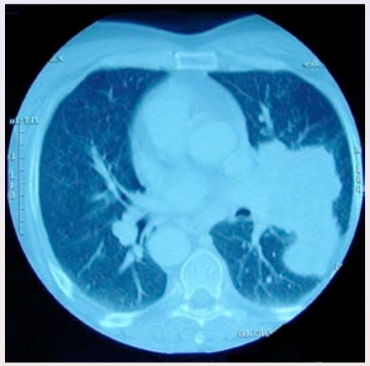


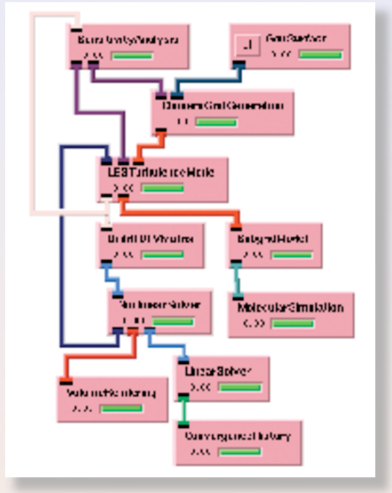
Figure modified from J. van Wijk, IEEE Vis 2005

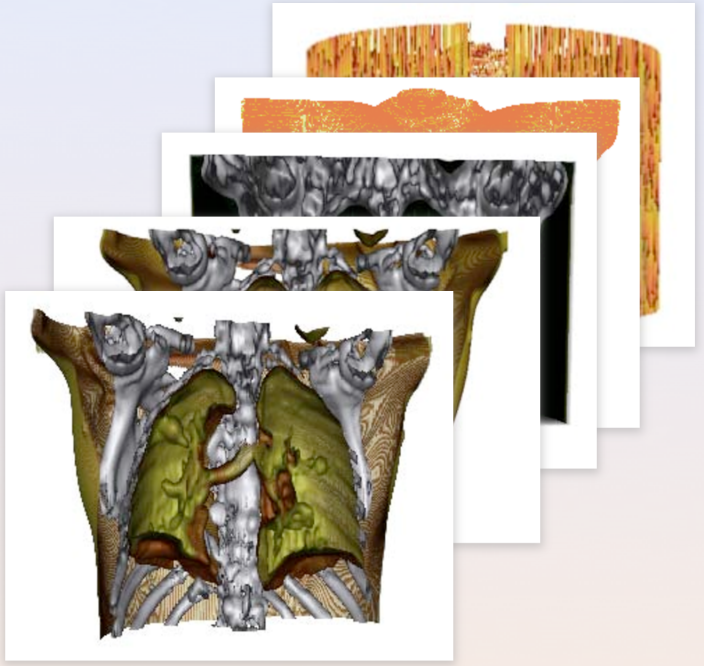
Data Exploration and Workflows

raw data: CT scan



workflow





Files (workflow specifications)

- anon4877_voxel_scale_1_zspace_20060331.srn
- anon4877_textureshading_20060331.srn
- anon4877_textureshading_plane0_20060331.srn
- anon4877_goodxferfunction_20060331.srn
- anon4877_lesion_20060331.srn

Notes

- Initial visualization wi
- Added texture an
- Added plane to vi i s
- Found good t f
- Identified lesion tissue

Exploration and Creativity Support

- Exploratory processes require reflective reasoning
- "*Reflective reasoning requires the ability to store temporary results, to make inferences from stored knowledge, and to follow chains of reasoning backward and forward, sometimes backtracking when a promising line of thought proves to be unfruitful. ...the process is slow and laborious*"

  Donald A. Norman
- Need external aids—tools to facilitate this process
  - Creativity support tools [Shneiderman, CACM 2002]
- Need aid from people—collaboration

Data Exploration and Workflows: Issues

- Hard to assemble and iteratively refine workflows
- Combine many tools and libraries: Need in-depth knowledge to weave them together
- No support for reflective reasoning
  - E.g., history of the exploration trail maintained manually through file-naming conventions and detailed notes
  - Hard to understand the exploratory process and relationships among workflows
- Lack of support for collaboration

Existing systems fail to provide the necessary infrastructure for exploratory tasks. As a result, the generation and maintenance of workflows is a major bottleneck in the scientific process

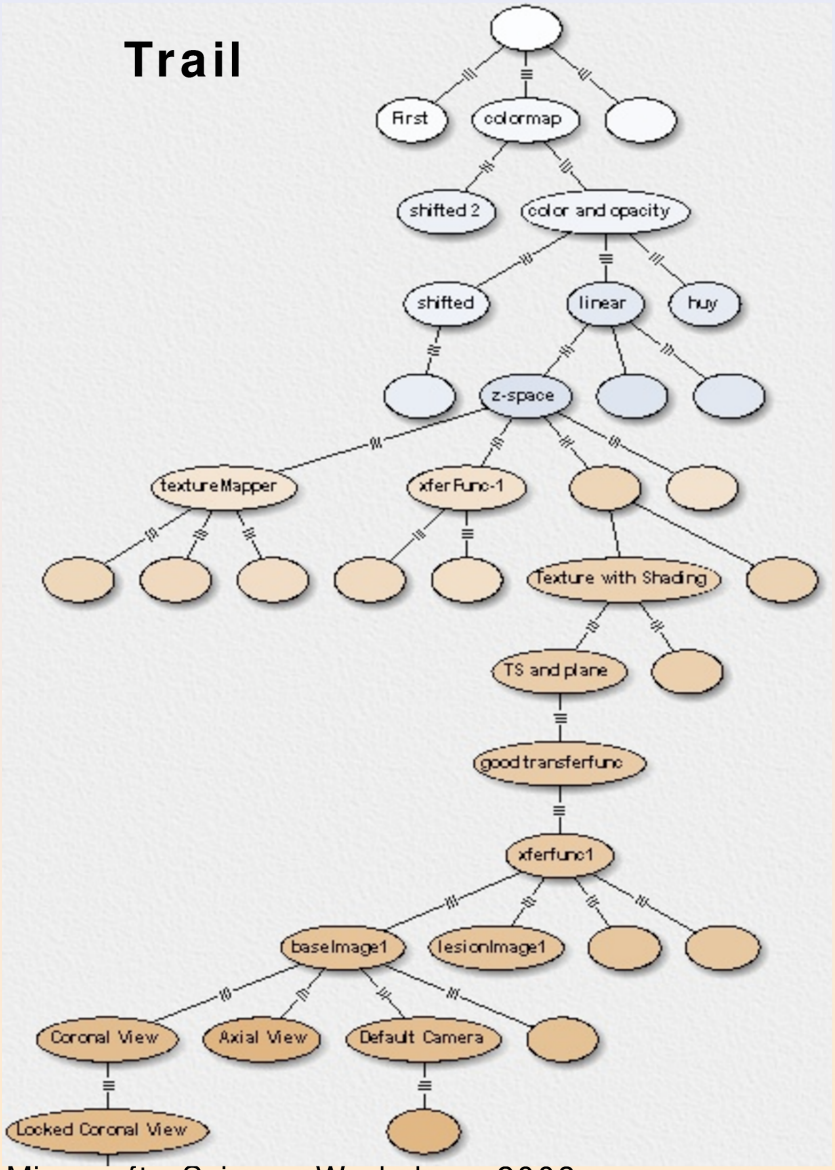
VisTrails: Managing Scientific Exploration

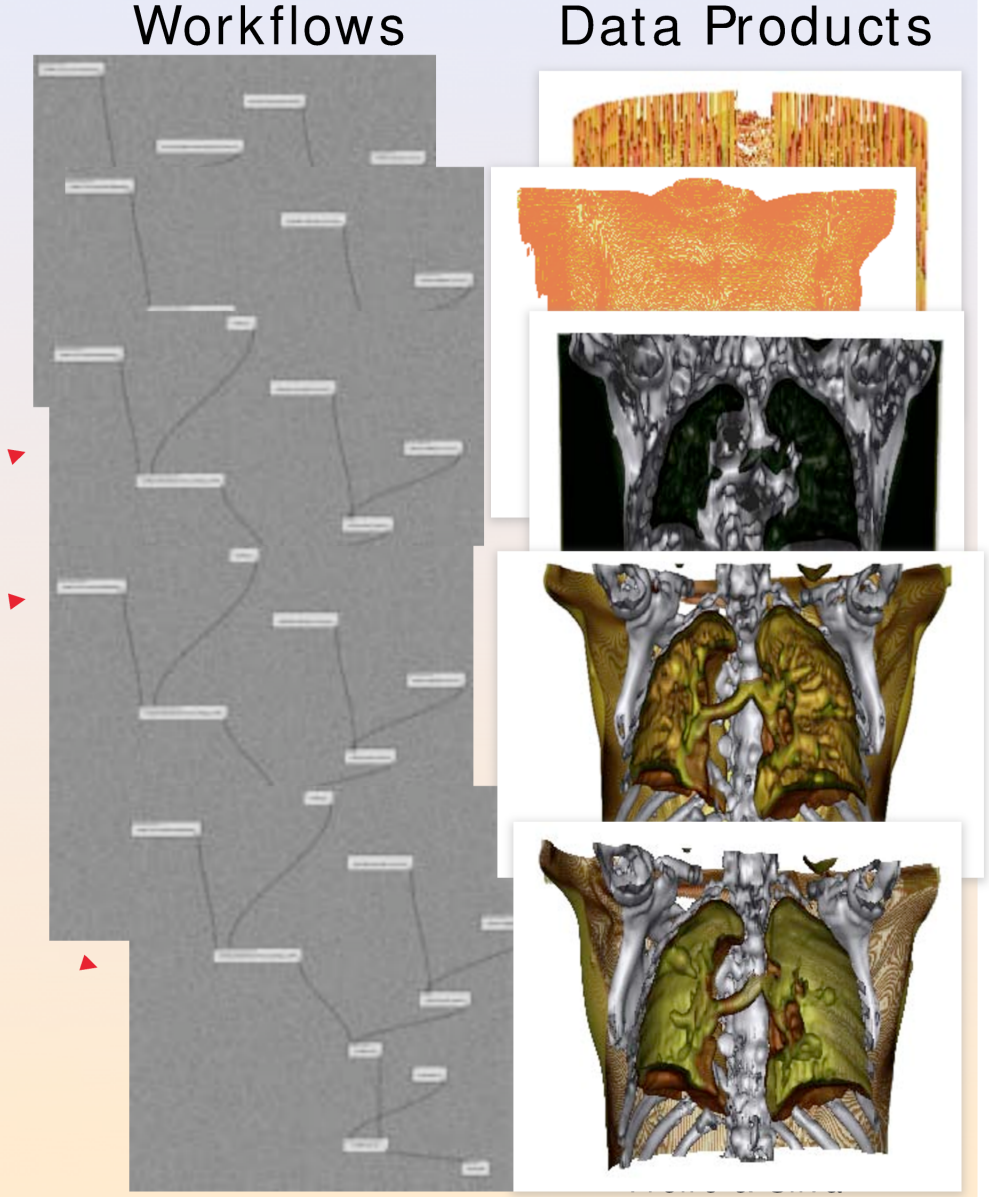
- Goal: reduce time to insight
- Build infrastructure to streamline *exploratory tasks* such as data analysis and visualization
- Support for *collaboration*
- *Usability*—provide tools and intuitive interfaces
- The VisTrails System: an open-source provenance-enabled scientific workflow system
  - > 6,000 downloads since 2007
  - Used in many applications: environmental modeling (OHSU), physics simulation (Cornell, LANL), medical studies (University of Utah), ...

Outline

- Using provenance to support reflective reasoning
- Exploring and re-using provenance
  - Querying workflows by example
  - Creating workflows by analogy
  - Auto-completion for workflows
- Emerging applications
- Future work

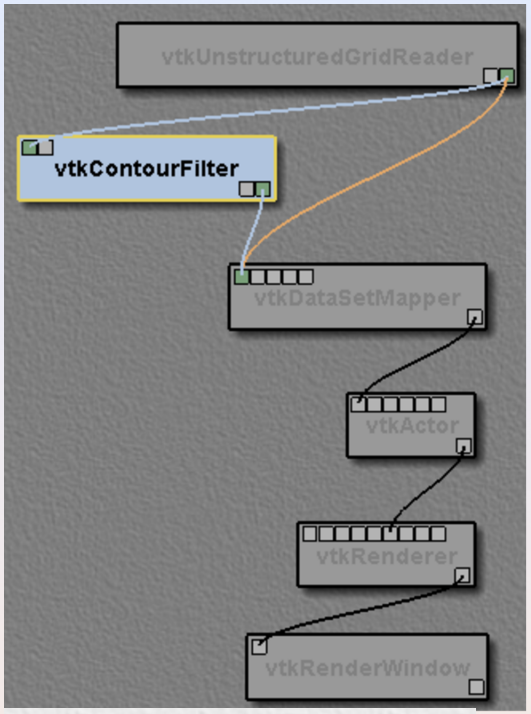
Keeping Exploration Trails





Change-Based Provenance

- Captures provenance of workflow evolution
- Records user actions
- Provenance = changes to computational tasks
  - Add a module, add a connection, change a parameter value



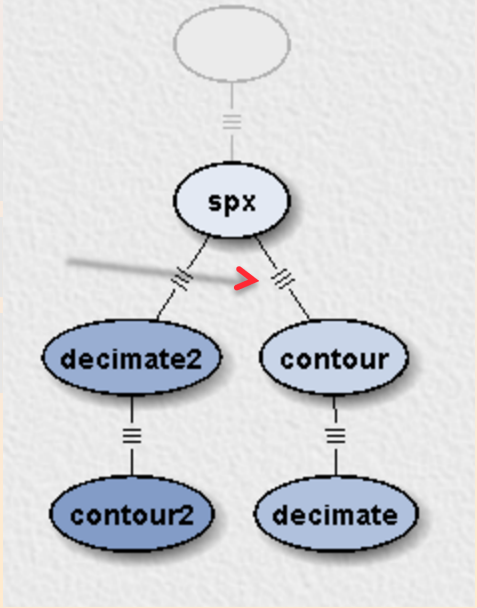
addModule

deleteConnection

addConnection

addConnection

setParameter



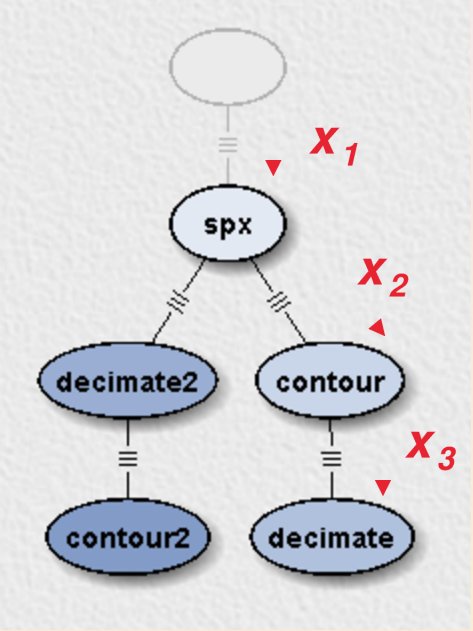
Change-Based Provenance

- Records user actions
- Provenance = changes to computational tasks
  - Add a module, add a connection, change a parameter value
- Extensible *change* algebra
- A *vistrail* node v_t corresponds to the workflow that is constructed by the sequence of actions from the root to v_t

$$v_t = x_n \circ x_{n-1} \circ \ldots \circ x_1 \circ \emptyset$$

[Freire et al, IPAW 2006]

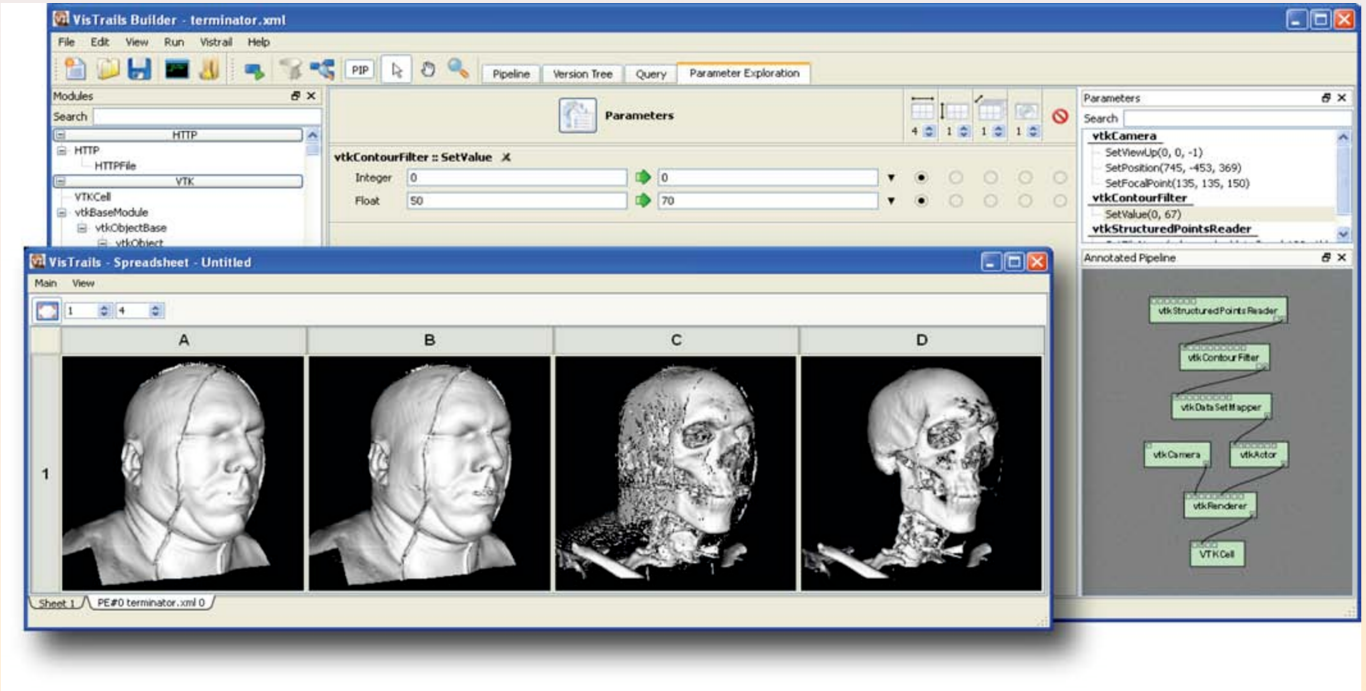
vistrail



Exploring the Change Space

- Scripting workflows: Parameter explorations are simple to specify and apply
- Exploration of parameter space for a workflow v_t

$(setParameter(id_n, value_n) \circ \ldots \circ (setParameter(id_1, value_1) \circ v_t)$



Exploring the Change Space

- Scripting workflows: Parameter explorations are simple to specify and apply
- Exploration of parameter space for a workflow $\boldsymbol{v_t}$

$$(setParameter(id_n, value_n) \circ \ldots \circ (setParameter(id_1, value_1) \circ \boldsymbol{v_t})$$

- Exploration of multiple workflow specifications

$$(addModule(id_i, \ldots) \circ (deleteModule(id_i) \circ \boldsymbol{v_1})$$

$$\ldots$$

$$(addModule(id_i, \ldots) \circ (deleteModule(id_i) \circ \boldsymbol{v_n})$$

- Results can be conveniently compared in the VisTrails spreadsheet
- Can create animations too!
- Caching to avoid redundant computations [Bavoil et al., IEEE Vis 2005]

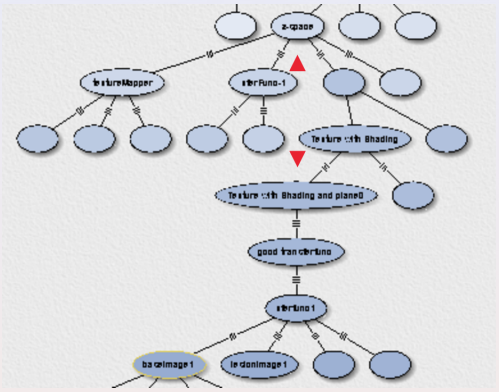
Computing Workflow Differences

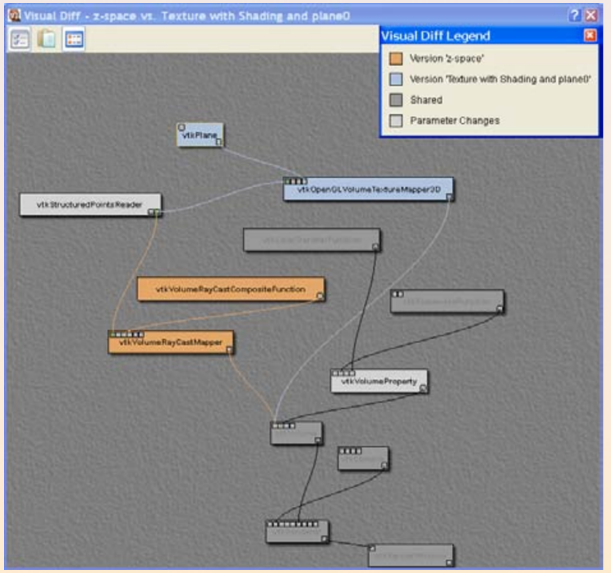
- No need to compute subgraph isomorphism!
- A vistrail is a rooted tree: all nodes have a common ancestor—diffs are well-defined and *simple to compute*

$vt_1 = x_i \circ x_{i-1} \circ \ldots \circ x_1 \circ \emptyset$

$vt_2 = x_j \circ x_{j-1} \circ \ldots \circ x_1 \circ \emptyset$

$vt_1\text{-}vt_2 = \{ x_i, x_{i-1}, \ldots, x_1, \emptyset\} - \{ x_j, x_{j-1}, \ldots, x_1, \emptyset\}$





- Different semantics:
  - Exact, based on ids
  - Approximate, based on module signatures

Collaborative Exploration

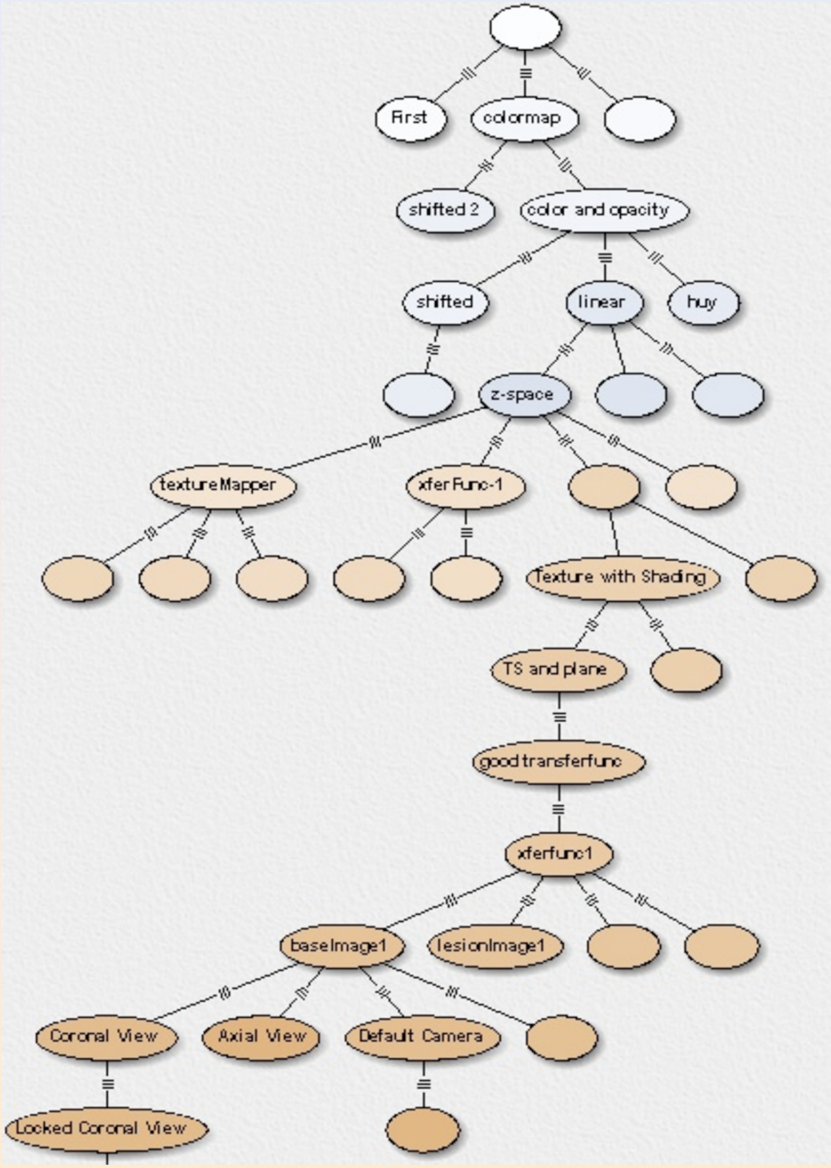
- Collaboration is key to data exploration
  - Translational, integrative approaches to science
- Store provenance information in a database
- Synchronize concurrent updates through locking
  - Real-time collaboration [Ellkvist et al., IPAW 2008]
- Asynchronous access: similar to version control systems
  - Check out, work offline, synchronize
  - Users exchange patches
- Synchronization is simple—provenance is monotonic
- No need for a central repository—support for distributed collaboration
  - For details see Callahan et al, SCI Institute Technical Report, No. UUSCI-2006-016 2006

Change-Based Provenance: Summary

- General: Works with any system that has undo/redo!
- Concise representation
- Uniformly captures data and workflow provenance
  - Data provenance: where does a specific data product come from?
  - Workflow evolution: how has workflow structure changed over time?
- Results can be reproduced
- *Detailed information about the exploration process*
- Provenance beyond reproducibility:
  - Support for reflective reasoning
  - Scalable exploration of the parameter space—results can be compared side-by-side in the spreadsheet
  - Support for collaboration
  - Understand problem-solving strategies—knowledge re-use

Exploring and Re-Using Provenance

- Storing detailed information is important, but not enough!
- Need appropriate user interface and operations to leverage information
  - Understand and re-use the history
- Simplify the creation of new workflows



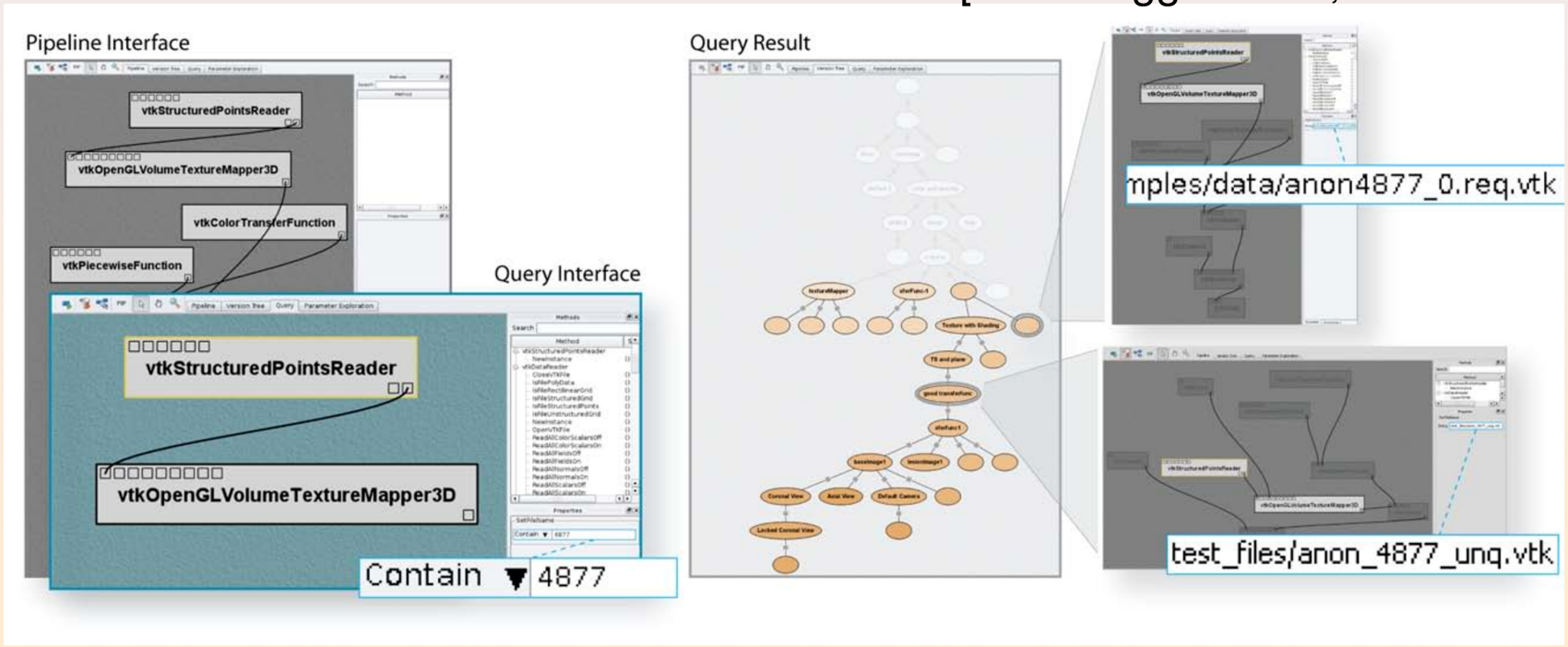
Looking for Examples

- Need to query workflow collection:
  - Find workflows that process a particular type of file
  - Find workflows that output a particular data product
  - Find workflows that contain a given module or sequence of modules
- Workflow are graphs: hard to specify queries using text
  - SQL, SparQL, Prolog…

Querying Workflows by Example

- WYSIWYQ -- What You See Is What You Query
- Interface to create workflow is same as to query

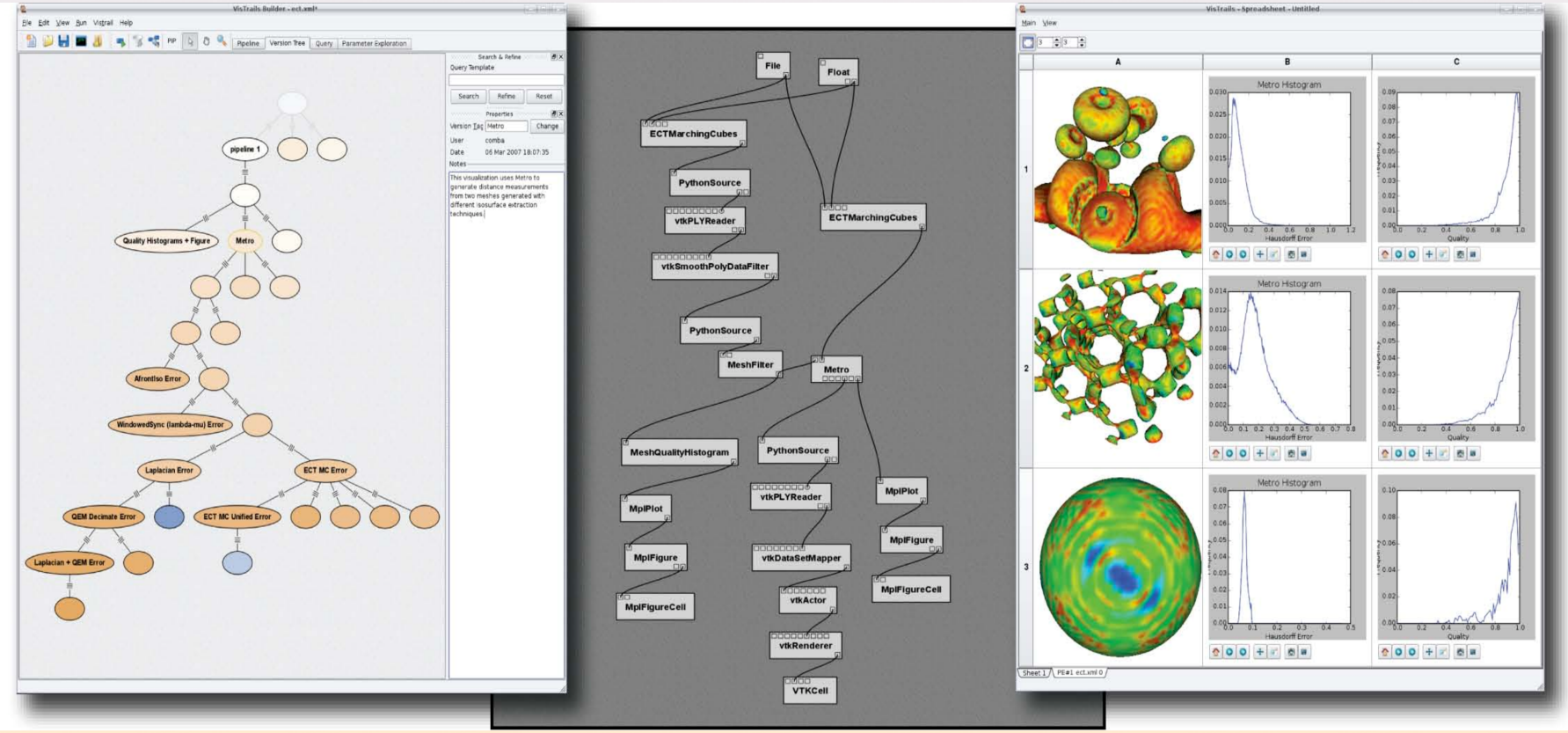
[Scheidegger et al., TVCG 2007



Refining Workflows

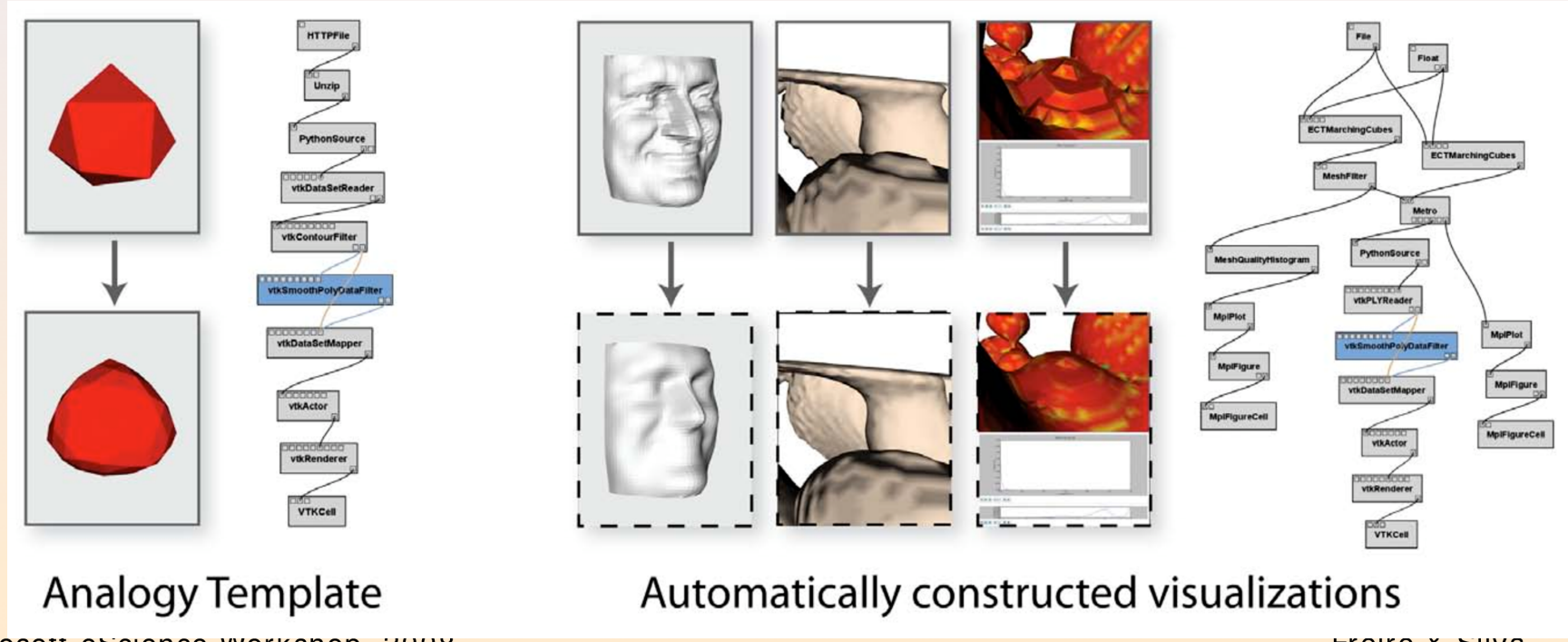
- Complex workflows are hard to create
  - Domain knowledge
  - Familiarity with different tools

Steep learning curve

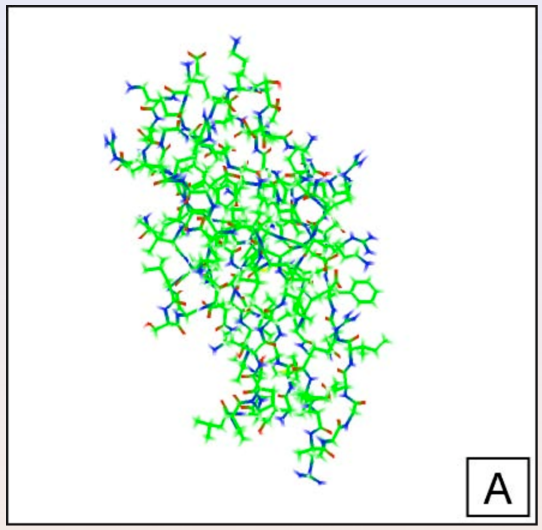


Refining Workflows by Analogy

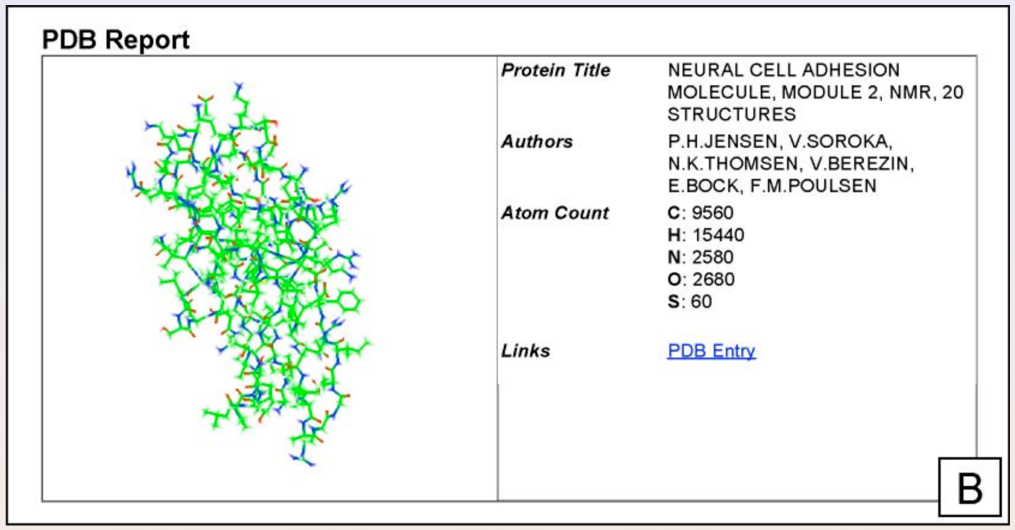
- Leverage the wisdom of the crowds in *shared provenance*
  - Some workflow refinements are common, e.g., change the rendering technique, publish image on the Web
- Apply refinements by analogy, automatically
  [Scheidegger et al, IEEE TVCG 2007]



Refining Workflows by Analogy



is to



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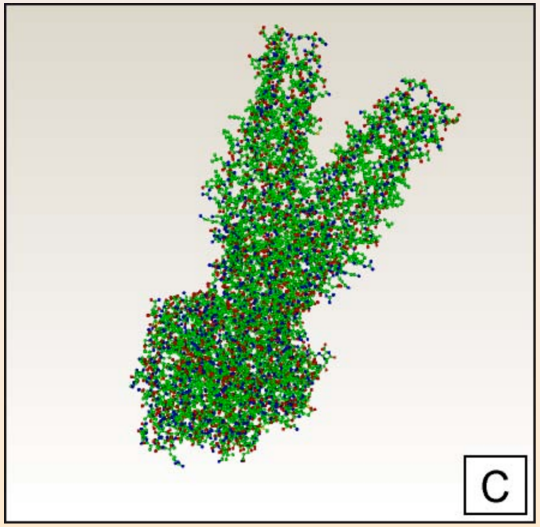
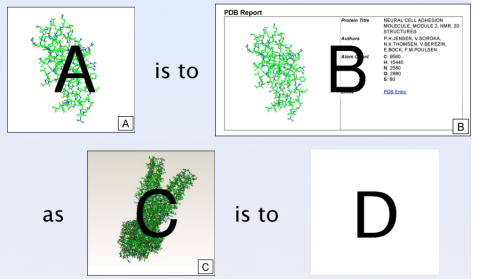


is to

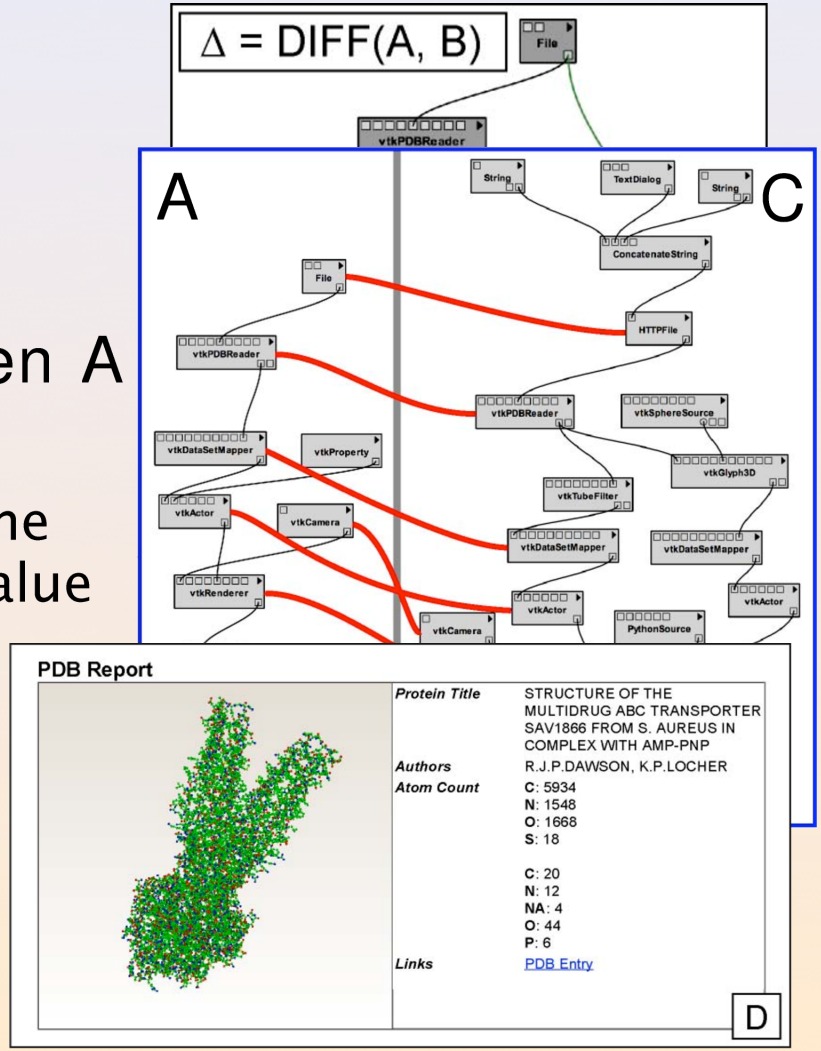
?

The Analogy Algorithm



1. Compute difference: Δ(A,B)
   - Just like a patch!
   - But…

   D = Δ(A,B) ◦ C may not be a valid workflow
2. Find correspondences between A and C: map(A,C)
   - Diffuse similarity scores across the product graph AxC using Eigenvalue decompositions
3. Compute mapped difference $\Delta_{AC}(A,B) = map(A,C)\ \Delta(A,B)$
4. D = $\Delta_{AC}(A,B) \circ C$



The Analogy Operation

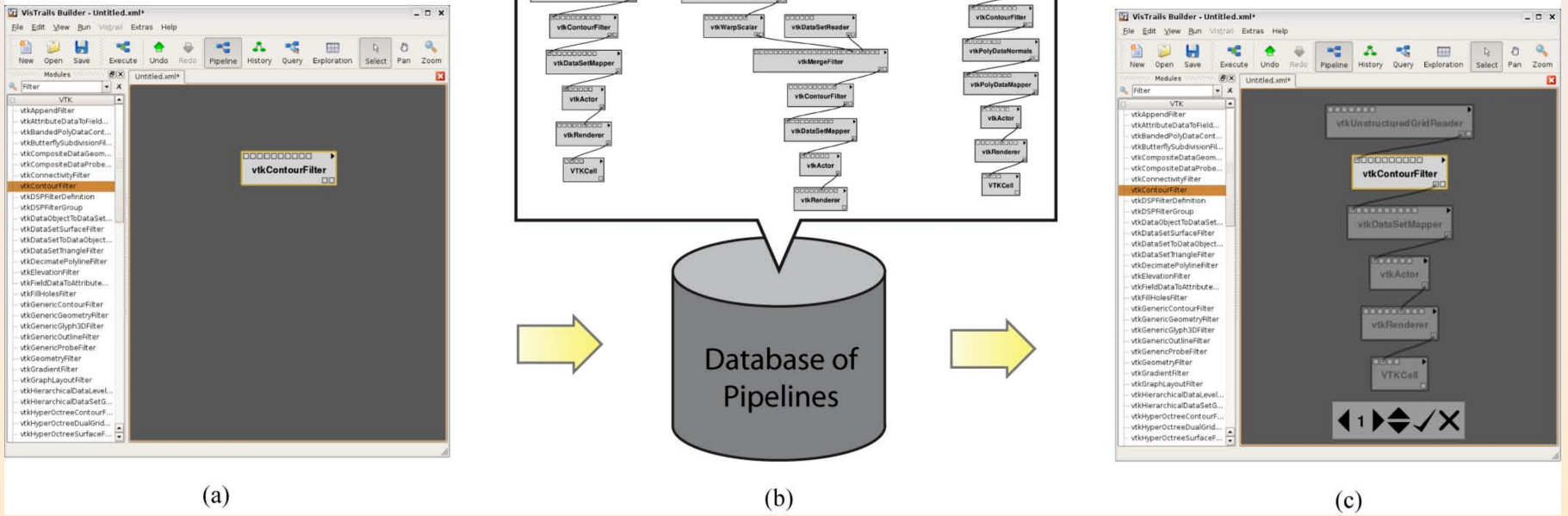
- Allows workflows to be refined without requiring users to directly modify the specification
- Basis for scalable updates
  - Analogies are not foolproof
    - If it works, great. If it doesn't, it may help
    - User can edit and fix the new version
  - Improve by
    - Using domain knowledge
    - Learning from user feedback

The Need for Guidance in Workflow Design

VisComplete: A Workflow Recommendation System

- Mine provenance collection: Identify graph fragments that co-occur in a collection of workflows
- Predict sets of likely workflow additions to a given partial workflow
- Similar to a Web browser suggesting URL completions

[Koop et al., IEEE Vis 2008]



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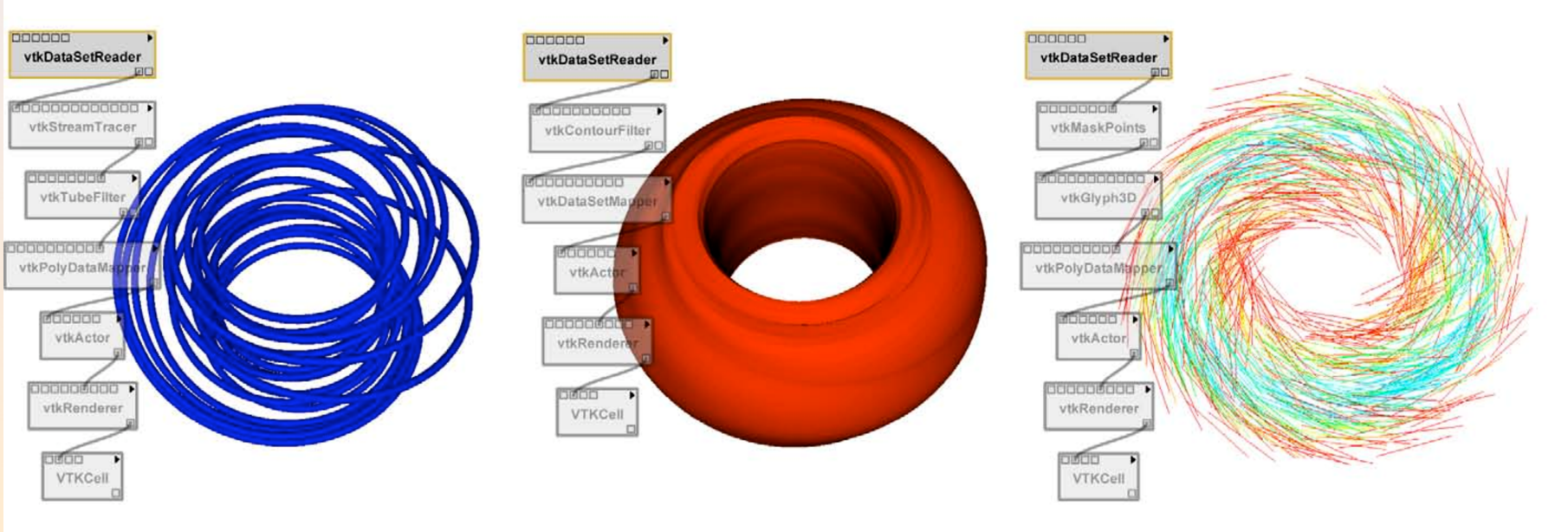

VisComplete: Demo

http://www.cs.utah.edu/~juliana/videos/viscomplete_h_264.mov

[Koop et al., IEEE Vis2008]

Results Summary

- Eliminates over **50%** of actions
- Selected completions are almost always in the first **four** suggestions
- A database of simple pipelines can aid users constructing more complex pipelines
- See [Koop et al., TVCG 2008] for details on how the path database is constructed and on the completion algorithm

Conclusions and Future Work

- Appropriate support for exploratory tasks is essential for a wider adoption and more effective use of scientific workflow systems
- Provenance can be used to support reflective reasoning
- Intuitive interfaces for simplifying the construction and refinement of workflows
- Sharing workflows provenance at a large scale creates new opportunities
  - Workflow/provenance repositories; provenance-enabled publications
  - Scientists can learn by example; expedite their scientific training; and potentially reduce their time to insight [Freire and Silva, CHI SDA, 2008]

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  - Huy T. Vo
  - Geoff Draper

For more info about VisTrails

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